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Machine Learning for Lattice QCD Simulations on Classical and Quantum Computers

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1 Introduction

In lattice QCD simulations, a large number of observables are calculated as expectation values over Gibbs ensembles of gluon fields (called lattices) generated using Monte Carlo Markov Chain methods with importance sampling using the Boltzmann weight. In modern lattice QCD simulations, computational costs for calculating and storing those observables are expensive. However, the fluctuations of various observables over the statistical samples of background lattices on a given ensemble are correlated. By exploiting the correlation between them, one can reduce computational and storage costs for lattice QCD calculations. Such exploitation of correlations is a problem well suited for machine learning (ML) algorithms as described in this LOI, and has the potential to significantly improve the precision of expensive lattice QCD calculations.

2 Machine learning regression algorithm predicting lattice QCD observables

Among the lattice QCD observables measured in the simulations, some observables are computationally cheap, while some observables are computationally expensive to calculate. If the correlation between the observables is high, one can build a machine learning regression algorithm that predicts the values of the computationally expensive observables from the values of the computationally

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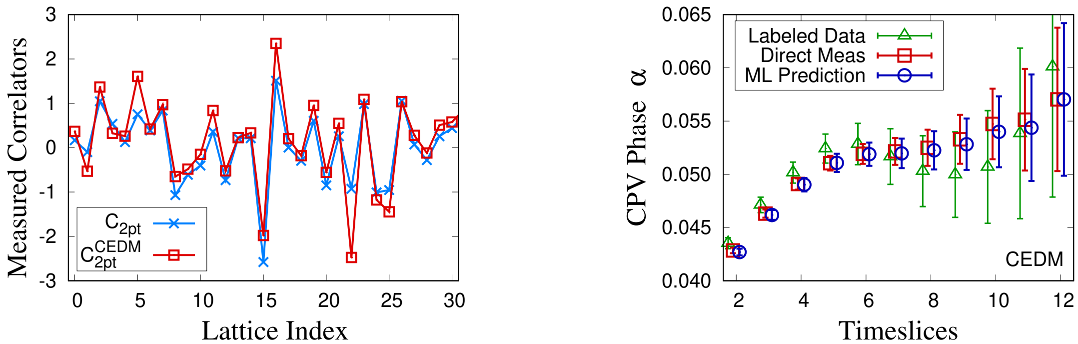

Figure 1: (Left) Normalized $C_{2\mathrm{pt}}^{\mathrm{CEDM}}$ and $C_{2\mathrm{pt}}$ on each lattice. (Right) Phase of neutron mass induced by CEDM calculated from direct lattice QCD measurements (□) and ML predictions (○)[1].

cheap ones for each lattice configuration. In Refs.[1,2], this idea has been demonstrated for a small class of the lattice QCD observables, along with a complete bias correction procedure that makes the final estimates unbiased and statistically sound. The results were promising. One example of the correlation and prediction is of the charge-parity violating (CPV) phase α of the neutron spinor in the calculation of the electric dipole moment (EDM) induced by quark chromo-EDM (CEDM) operator is shown in Figure 1. The proposed algorithm can be applied to any lattice QCD calculations, so we propose to explore a larger class of observables that exhibits strong correlations for the application of the method. Also, the proof-of-principal studies used only simple ML regression models. We will investigate a wide range of machine learning algorithms to improve prediction quality.

3 Quantum Machine Learning for Lattice QCD

Sparse coding refers to a class of unsupervised ML algorithms for finding an optimized set of basis vectors and the fewest number of non-zero coefficients accurately reconstructing inputs vectors. Recently, a mapping of the sparse coding to the D-Wave system is proposed and showed good utilization of the quantum annealing features of the D-Wave system[3]. In Ref.[4], we developed a machine learning regression algorithm utilizing the D-Wave quantum annealer based on the sparse coding and applied it to the prediction of lattice QCD observables. The results are promising, yet, current performance is limited by the total number of qubits available. Further improvements of the algorithm along with hardware developments will increase performance and extend the method to a wider range of applications.

The sparse coding is a natural feature extraction and dimensional reduction algorithm, and quantum implementation of the sparse coding is a way to accelerate the computational cost for ML training and prediction. Application of the sparse coding on experimental and simulation data will yield algorithms for data compression and computational cost reduction.

References

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